National Center for Computational Sciences Snapshot
The week of November 6, 2006

Science Highlight – Building Nuclei from the Ground Up

A team of nuclear physicists led by David Dean of Oak Ridge National Laboratory (ORNL) and the University of Tennessee is using physics to build nuclei from the ground up. As a part of Dean's LCF Project "Ab-initio Nuclear Structure Computations," the researchers are undertaking the ambitious task of putting together the microscopic nuclear physics of the atom into a theoretical model that accurately predicts the mass, shape, size, and basic energy spectrum of intermediate-mass elements such as oxygen and calcium. The nuclear properties that such models can reveal are crucial factors in the study of nuclear fusion and fission. Therefore, they are vital pieces in the questions of how stars burn and where the elements in our universe were formed.

Nuclear physicists in the atom construction business work to develop the simplest possible blueprints for determining the quantum mechanical behavior of the nucleus that still give results accurate enough to match experiments. To strike this balance, Dean's research team is using a technique called the Coupled Cluster approach, which uses a set of coupled nonlinear algebraic equations to describe the interactions of the nuclear particles. The technique has already been well established and is widely used in quantum chemistry. Its framework allows Dean's team to explore the roles of both two- and three-body forces in intermediate-mass nuclei, something that has never been successfully attempted for such massive nuclei. The complexity that comes with adding the three-body force pushes the numerical solution for the problem past the solving capacity of most computers. For example, the calculations for oxygen-16 require the solution of 16 trillion coupled nonlinear equations. Numerical solutions of this magnitude require supercomputing resources. The team is using the National Center for Computational Sciences' (NCCS's) Cray XT3 (Jaguar) supercomputer in its research.

The group has preliminary results for oxygen-16 that qualitatively match with experimental data, but more detailed calculations must be done before the team is satisfied that the technique is truly working. In another year, the researchers hope to tackle the much more complex calcium-40 nucleus. The team does not believe that the model can be used for nuclei with more than 100 nucleons because of the extreme complexity contained in such massive systems. The models that Dean's collaboration are developing will help atom builders understand which physics must be treated fully and which physics can be approximated. Their approach will eventually be used to validate simpler schemes that require less computational resources and can therefore model more massive nuclei.

Research team member Thomas Papenbrock says, "If it is really possible to build a calcium-40 from scratch, using two- and three-body forces to create a model that gives a reasonable agreement with experiment, this would be a huge step forward." Each of these models is a step toward calculating the nuclear properties for species on the nuclear chart that cannot be probed experimentally.

2006 Fall Creek Falls Conference

The 2006 Fall Creek Falls Conference was held October 22–24. The annual workshop is collaboration between the NCCS and ORNL's university partners (Duke University, Georgia Institute of Technology, Florida State University, North Carolina State University, University of Virginia, Virginia Polytechnic Institute and State University, and the University of Tennessee). This annual workshop brings national and international leaders from a variety of scientific disciplines together with NCCS users, ORNL staff, and faculty and graduate students from the university partners to discuss the latest developments in scientific and engineering research.

The theme for the 2006 conference was *Computational Science at the Petascale*. Notable scientists from across the country discussed the progress and challenges of high-performance computing on petascale machines. Speakers from several applications communities discussed the software and hardware issues surrounding science at the petascale. ORNL personnel gave several presentations focusing on the future of high-performance computing and the challenges that must be overcome as petascale applications become a reality.

Notable climatologist Warren Washington of the National Center for Atmospheric Research gave a presentation entitled "Petascale Modeling the Climate of the 20th and 21st Centuries: Recent Results." In it, he indicated that climate researchers will use petascale computing to predict future climates based on scenarios of anthropogenic emissions and changes resulting from options in energy policy. Following the conference, Washington and several other scientists came to ORNL and toured the NCCS facilities.

NCCS Facilities

The work on the second floor of the Computational Sciences Building at ORNL has been completed on schedule and within budget. The startup and testing of the power distribution and HVAC units has been completed, and the chilled water loop has been tied into the main chilled water system. In addition, the ceiling lights, emergency lights, fire protection horns and strobes, public address system, smoke detection system, and signage are all being finalized this week.

The construction is taking place to ready the facility to house an additional 68 cabinets, arriving next week, for Jaguar. The machine will be upgraded to 100 teraflops in early 2007 and ultimately to 250 teraflops in late 2007. The completion of the current construction is an important step on the path to deliver the petascale machine by late 2008.

1st Annual Cray Technical Workshop Announced

Cray, Inc., and ORNL are hosting the first annual American Cray Technical Workshop at the Gaylord Opryland Hotel in Nashville, Tennessee. The workshop, which will take place February 26–28, 2007, is modeled after similar programs sponsored by Cray Europe in which European users discuss their work on various Cray architectures.

The workshop will address the numerous advances made on the Cray XT3 in the past year, resulting in 20–30 applications currently sustaining 1 teraflops in performance. There will be several talks from Cray staff and discussion of future Cray architectures. Members from the user community are being asked to present their successful experiences and discuss any particular challenges or difficulties overcome in achieving those successes.

The program will begin with a tutorial Monday morning, February 26, by John Levesque on the optimization of the Dual Core XT3. The talks from the user community and selected Cray staff will be given from Monday afternoon through Wednesday, February 28.

A registration site is set-up at http://nccs.gov/news/workshops/cray/.